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| Autore | Bulatov Vasily V |
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| ISBN | 0-19-191661-7 1-280-96503-7 0-19-151366-0 1-4294-5992-1 |
| Descrizione fisica | 1 online resource (301 p.) |
| Collana | Oxford series on materials modelling ; ; 3 |
| Altri autori (Persone) | CaiWei <1977-> |
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| Soggetti | Dislocations in crystals - Computer simulation Electronic books. |
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| Nota di bibliografia | Includes bibliographical references (p. [275]-280) and index. |
| Nota di contenuto | Contents; 1 Introduction to Crystal Dislocations; 1.1 Perfect Crystal Structures; 1.2 The Concept of Crystal Dislocations; 1.3 Motion of a Crystal Dislocation; I: ATOMISTIC MODELS; 2 Fundamentals of Atomistic Simulations; 3 Case Study of Static Simulation; 4 Case Study of Dynamic Simulation; 5 More about Periodic Boundary Conditions; 6 Free-energy Calculations; 7 Finding Transition Pathways; II: CONTINUUM MODELS; 8 Peierls-Nabarro Model of Dislocations; 9 Kinetic Monte Carlo Method; 10 Line Dislocation Dynamics; 11 Phase Field Method; Bibliography; Subject Index; A; B; C; D; E; F; G; H; I; K LM; O; P; R; S; T; V; W; Y; Z |
| Sommario/riassunto | Presenting a variety of methods for computer simulations of crystal defects in the form of 'numerical recipes', complete with computer codes and analysis tools, this text provides a useful starter kit for further method development in the computational materials sciences. |